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Andersen, Jørgen Vitting; Jensen, Henrik Jeldtoft; Mouritsen, Ole G.

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Crossover in the power spectrum of a driven diffusive lattice-gas model

Jørgen Vitting Andersen
Department of Structural Properties of Materials, The Technical University of Denmark, Building 307, DK-2800 Lyngby, Denmark

Henrik Jeldtoft Jensen
Nordisk Institut for Teoretisk Fysik (NORDITA), Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark

Ole G. Mouritsen
Department of Structural Properties of Materials and Department of Physical Chemistry, The Technical University of Denmark, Building 307, DK-2800 Lyngby, Denmark

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A driven diffusive lattice-gas model with stochastic dynamics is used to study, via a Monte Carlo simulation, the fluctuations in the particle density and the lifetime of the particles in the system. The scaling properties of the power spectrum $S(f)$ and the lifetime distribution function $D(t)$ exhibit a crossover from $(1/f^{\beta})$- to $(1/f^2)$-noise behavior, with $\beta \simeq 1.5$, when the drive is sufficiently strong to induce a characteristic time scale. We argue that the scaling behavior with $\beta \simeq 1.5$ is governed by the stochastic nature of the dynamics, whereas deterministic dynamics leads to $\beta \simeq 1$.

The introduction of the concept of self-organized criticality[1] has inspired studies of $1/f$ noise, especially by use of computer simulations.[2,3] Systems which are discrete in both time and space are particularly useful for such studies since one can afford to follow the evolution of these systems over the very long time intervals that are required for determining the low-frequency behavior of the power spectra. It is of interest to investigate the power spectra of quantities with a simple physical interpretation. An example of such a study is the simulations in Ref. 2 of a deterministic lattice-gas cellular-automaton model of flux flow in type-II superconductors. In that work, the power spectrum for the total number of particles in the system was found to behave as $1/f^{\beta}$ with $\beta \simeq 1$. The fundamental property of systems exhibiting $1/f$ noise is the absence of any characteristic time scale. Obviously it is of interest to study the crossover properties of the power spectra as either a stochastic dynamics is introduced or as a time scale is made to establish itself.

In the present paper, we present the results of Monte Carlo simulations on a lattice-gas model of a driven diffusive system which is well suited to study crossover behavior in the power spectrum. The model has stochastic dynamics induced by thermal fluctuations. A time scale may be introduced via an external driving field. The model is associated with a Hamiltonian and we consider both attractive and repulsive interactions. Although we have considered the model in one, two, and three spatial dimensions, we concentrate on two dimensions. A particular dynamic boundary condition takes the role of a driving field which provides a mechanism for introducing a characteristic time scale in the dynamics.[4] Our main result is that the model displays a power spectrum, $S(f) \sim 1/f^{\beta}$, with $\beta \simeq 1.5$, independent of the temperature, provided that the drive is sufficiently weak and hence no characteristic time scale has established itself. When the drive is stronger and has introduced a characteristic time scale, we observe a crossover to $1/f^2$ noise. These results hold independent of the temperature, the nature of the interactions, and the spatial dimension. That it is the stochastic nature of the dynamics which governs the scaling behavior with $\beta \simeq 1.5$ is furthermore supported by our finding that the introduction of stochastic dynamics in the deterministic model of flux flow[2] associated with $\beta \simeq 1$ leads to a crossover to $\beta \simeq 1.5$. We show, in general, that if the particles on the lattice were independent random walkers, an exponent $\beta = \frac{3}{2}$ is expected from the scaling behavior (namely $t^{-3/2}$) of the first-return time of a random walker.

The model on which most of our results are based was recently proposed[4,5] as a model for describing the steady-state properties of a mass-transporting finite system in a chemical-potential gradient. The model is a kinetic lattice model defined on a two-dimensional rectangular lattice of $L \times M$ $(L > M)$ sites coupled by a nearest-neighbor local lattice-gas Hamiltonian

$$H = J \sum_{\langle i,j \rangle} n_i n_j , \tag{1}$$

where $n_i = 0,1$ is the occupation variable of the ith site and $J > 0$ and $J < 0$ for repulsive and attractive interactions, respectively. The lattice has periodic boundary conditions in the short dimension (M) and free boundaries in the long dimension (L). Hence, the system is characterized by a bulk part and a surface (the two edges) made up of rows 1 and L. The dynamics of the model is a particle-conserving Kawasaki particle-hole exchange in the bulk allowing for exchanges between nearest- and next-nearest-neighbor sites, combined with Glauber particle creation and/or annihilation at the edges. Thus, the total number of particles, $N(t)$, on the lattice is not conserved but fluctuates in time t. The time is measured in units of Monte Carlo steps per site. The system dynamics are simulated by standard Metropolis Monte Carlo sampling corresponding to thermal noise in the bulk. The model may be driven dynamically into a particle-transporting nonequilibrium steady state[4] by introducing an E field which acts between rows 1 and 2 and between rows $L-1$ and L. Whenever a particle exchange is attempted between these rows, an extra term,

$$p=\min[1,\exp(-\Delta H-\epsilon E)/k_BT]\,, \qquad (2)$$

enters the Metropolis transition probability for going from one configuration to the next. ΔH is the associated energy change and $\epsilon=-1,0,+1$ depending on whether the particle jumps along, transverse to, or against the direction of the E field. Since the E field is chosen to be along the long dimension of the lattice, the steady state is controlled by a mass flux where particles are pumped into the system at one edge and pumped out at the other edge. This model, which recently was applied to study diffusion-controlled oxygen ordering in finite samples of high-T_c superconductors of the $YBa_2Cu_3O_{7-\delta}$ type,[6] is related to a general class of driven diffusive systems which have attracted considerable attention due to their interesting nonequilibrium critical behavior.[7,8]

The properties of the model are calculated by standard Monte Carlo simulation techniques. In particular, we have calculated the distribution, $D(t)$, of lifetimes for particles on the lattice and the temporal variation of the total particle number $N(t)$. The power spectrum $S(f)$ is then obtained as the square modulus of the Fourier transform of $N(t)$. The simulations are carried out on different lattice sizes and for different strengths of the driving field E. Different temperatures above as well as below the kinetic phase transition[4] are considered and both the case of repulsive and attractive interactions are studied. Since the general results for the attractive and repulsive interactions are qualitatively similar, we shall only describe in detail the repulsive case. In the following, the driving field E is given in units of J and the temperature in units of the transition temperature for the equilibrium system, $k_BT_c/J\simeq 0.57$. For each set of parameters, the simulation results are averaged over 20 independent runs, each representing a time duration in the steady state of 10^5 Monte Carlo steps per lattice site.

Figures 1 and 2 show the power spectra and the lifetime distributions for a high temperature, $T=3T_c$, and a relatively weak driving field, $E/J=1$, in the case of three different lattice sizes. The crossover in $S(f)$ at small frequencies (or long times) to white noise is a finite-size effect. The correlation between $N(t)$ and $N(t+\tau)$ simply vanishes when τ becomes larger than the maximum time a particle spends on the lattice. This maximum time is determined by the finite size of the lattice in the transporting direction. The data of Figs. 1 and 2 show that the power spectrum and the lifetime distribution function both display power-law scaling

$$S(f)\sim f^{-\beta},\; D(t)\sim t^{-\alpha}, \qquad (3)$$

with exponent values $\beta\simeq 1.5$ and $\alpha\simeq 1.5$. Hence, the scaling relation,[9] $\alpha+\beta=3$, is approximately fulfilled.

The dependence upon the magnitude of the driving field is illustrated in Figs. 3 and 4 in the case of a low temperature, $T=\frac{1}{3}T_c$. It is important to notice that the exponents $\alpha\simeq\beta\simeq 1.5$ are also obtained in the absence of a driving field, $E=0$, in which case there is no net drift through the system. An increase in E leads to an increase in the particle current.[4] Figure 3 shows that the exponent β of the power spectrum $S(f)$ at this low temperature changes from 1.5 to 2 as E/J is increased above 0.5. At the same time, the scaling regime of $D(t)$ is diminished, which makes it increasingly difficult to define a scaling power. The part of the distribution which appears at short times before the system enters the scaling regime refers to the lifetimes of particles at the two edges. It is seen that $D(t)$ in the driven systems develops a broad-peak contribution at long lifetimes.[10] As E is increased, this contribution is enhanced, the scaling regime diminishes, and an effective cutoff in the distribution function manifests itself (see Fig. 4, curve e). The broad-peak contribution in $D(t)$ reflects the fact that the total mass flux is described by a center-of-mass velocity, $\langle v_x\rangle$, in the transporting direction. This contribution is therefore centered around $t\simeq L/\langle v_x\rangle$. The contribution is very broad because the system is only driven at the edges. For a diffusive system driven at every site,[7] a much more narrow distribution is

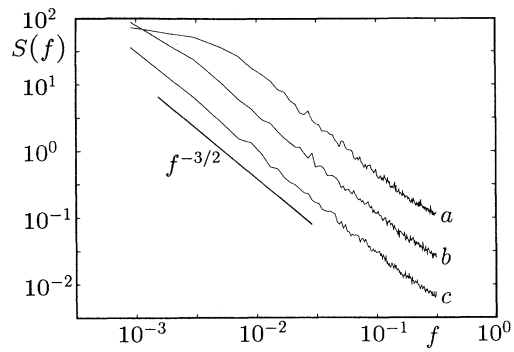

FIG. 1. Log-log plot of the power spectrum $S(f)$ for the model with repulsive interactions at a temperature $T=3T_c$ and driving field $E/J=1$. Results are shown for three different lattice sizes, $L\times M$, where L is in the transporting direction. Curve a, 50×10; curve b, 100×10; curve c, 200×10. The thick solid line corresponds to the relation $S(f)\sim f^{-1.5}$.

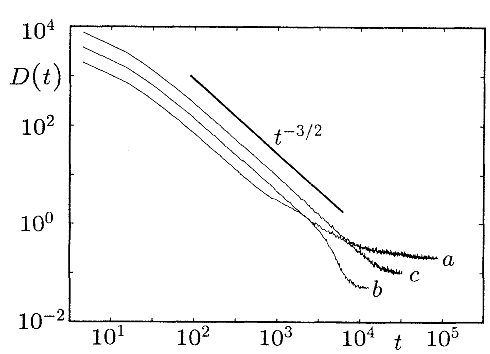

FIG. 2. Log-log plot of the distribution of lifetimes, $D(t)$, corresponding to Fig. 1. For the sake of clarity, the data have been multiplied by factors 1, 2, and 4 going from curve a to curve c. The thick solid line corresponds to the relation $D(t)\sim t^{-1.5}$.

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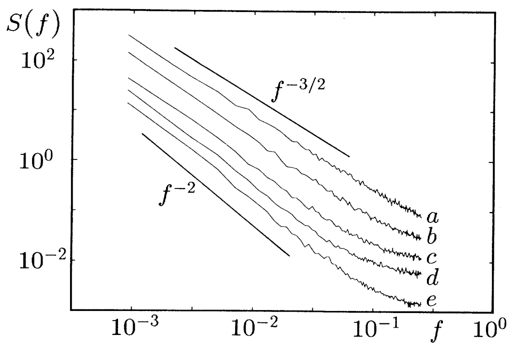

FIG. 3. Log-log plot of the power spectrum $S(f)$ for the model with repulsive interactions at a temperature $T=\frac{1}{3}T_c$ and different values of the driving field E/J. Curve a, $E/J=0$; curve b, $E/J=0.5$; curve c; $E=0.8$; curve d; $E=1$; curve e, $E=5$. The results refer to a lattice with $L\times M=200\times 10$ lattice sizes. For the sake of clarity, the data have been multiplied by factors 16, 8, 4, 2, and 1 going from curve a to curve e. The thick solid lines denote the relations $S(f)\sim f^{-\beta}$, with $\beta=1.5$ and 2, respectively.

expected which will reduce to a δ function when all particles have the same velocity. A distribution of lifetimes dominated by a peak centered about a characteristic lifetime leads to a $1/f^2$ power spectrum. This follows from the discussion in Ref. 9 where a random linear superposition of box signals was considered. If the lifetime of the individual box signals is distributed according to $D(t)$, the power spectrum of the linear superimposed signals is given by

$$S(f)=\frac{\nu}{(\pi f)^2}\int_0^\infty dt\, D(t)\sin^2(\pi f t)\,, \tag{4}$$

where ν is the rate with which the individual box signals are introduced. Hence, if $D(t)=\delta(t-t_0)$, the power spectrum reduces to $S(f)\propto \sin^2(\pi t_0 f)/f^2$. A small spread in the values of t_0 will wash out the oscillations from $\sin^2(\pi f t_0)$.

One may mistakenly relate the change in the exponent values directly to the increase in the particle flux. However, the flux only decreases about 8% in going from $E/J=5$ to 1 and about 20% in going from $E/J=5$ to 0.5.

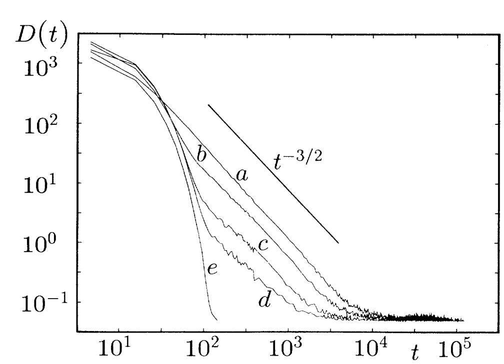

FIG. 4. Log-log plot of the distribution of lifetimes, $D(t)$, corresponding to Fig. 3. The thick solid line denotes the relation $D(t)\sim t^{-1.5}$.

Therefore, we rather associate the crossover to ($1/f^2$)-noise behavior in strongly driven systems to the effective emergence of a *characteristic time scale* in the dissipative dynamics. The characteristic time is the average time it takes a particle to get across the finite system. The effective cutoff is due to the thermal activation associated with the transition probabilities, Eq. (2). According to these probabilities, the particles experience the system edges as semipermeable barriers when the drive is strong. This leads to an effective gap in the spectrum of lifetimes (cf. Fig. 4) between the short-time contribution resulting from the particles at the two edges and the broad-peak contribution resulting from the center-of-mass movement. Hence, we are led to argue that it is not the mass flux as such which causes the crossover, but rather the very mechanism of the drive, Eq. (2), which introduces a characteristic time scale in the dynamics. This crossover from $1/f^{1.5}$ to $1/f^2$ noise is controlled by E/T rather than by E. Large values of E/T simply destroy the temporal scaling by introducing a characteristic time $L/\langle v_x\rangle$ leading to the exponent $\beta=2$.

We have found a similar crossover in the case of attractive interactions. The two cases only differ in the amplitudes of the scaling laws and the details of the crossover behavior. Since we consider an open system, the attractive case will at low temperatures lead to very high densities and therefore very long time scales and consequently a slower relaxation into the steady state. The exponents $\alpha\simeq 1.5$ and $\beta\simeq 1.5$ are also obtained for a noninteractive lattice gas, $J=0$. Moreover, the *same* behavior is found in both one and three dimensions.

Let us now turn to a discussion of the exponents α and β and the observed crossover behavior. It turns out that it is useful for this discussion to consider the ideal case of independent random walkers on a lattice.[11] We shall derive the properties of the lifetime distribution of such a system and then relate them to our diffusive driven system. We present the arguments for arbitrary spatial dimension. For independent random walkers, the total number of particles on the lattice is the sum of square-box signals:

$$N(t)=\sum_{\tau_i} n_{\Delta t_i}(t-\tau_i)\,, \tag{5}$$

where the box function $n_{\Delta t_i}$ contributes to $N(t)$ in the time interval $[\tau_i,\tau_i+\Delta t_i]$ during which particle number i is on the lattice. The function $n_{\Delta t_i}(t)$ is given by $n_{\Delta t_i}(t)=1$ if $t\in[0,\Delta t_i]$ and $n_{\Delta t_i}(t)=0$ otherwise. The power spectrum of such a superposition of independent signals started at random times was discussed in Ref. 9. It was shown that a scaling behavior of the distribution of lifetimes of the individual box signals of the form $D(t)\sim t^{-\alpha}$ leads to a power spectrum for $N(t)$ of the form $S(f)\sim f^{-\beta}$, where $\beta=3-\alpha$ for $\alpha>1$ and $\beta=2$ for $\alpha<1$.

The lifetime of the walkers on the lattice is the time spent from when they are introduced at one of the edges to when they are annihilated at either the left or the right edge. This time is given by the first-passage time of a walker started, say, at time $t=0$ with the x coordinate $x=L$ through one of the hyperplanes $x=0$ or $x=L+1$. The distribution of the first-passage time of a random walker, started at $t=0$ on the hyperplane $x=x_0$, through another hyperplane $x=x_1$, is in all dimensions given by[12]

$$D(t,R)=|R|[\delta t/4\pi\langle(\Delta s)^2\rangle t^3]^{1/2} \times\exp[(\langle s\rangle t/\delta t-R)^2/4\langle(\Delta s)^2\rangle t/\delta t]\ . \quad (6)$$

Here, $R=x_1-x_0$ and $\langle s\rangle$ is the average step size of the random walker. $\langle(\Delta s)^2\rangle$ is the variance of the step sizes, and δt is the time step. This distribution scales as $1/t^{3/2}$ when $(\langle s\rangle t/\delta t-R)^2/[4\langle(\Delta s)^2\rangle t/\delta t]\ll 1$, i.e., for $t\in[t_-, t_+]$. The two end points of this scaling interval depend on the ratio $\langle s\rangle/\langle(\Delta s)^2\rangle$ which measures the asymmetry of the random walk. For a symmetric walk, i.e., $\langle s\rangle=0$, we have $t_-=\delta tR^2/4\langle(\Delta s)^2\rangle$ and $t_+=\infty$. The scaling interval shrinks as the walk becomes more asymmetric and eventually vanishes with $t_-=t_+=\delta t|R|/\langle s\rangle$.

We can use these results for a system of independent random walkers to interpret the results of our simulations of the driven diffusive system. First, we note that the lattice-gas model displays power spectra and lifetime distribution functions with the same exponents as the random walkers, despite the fact that the particles in the lattice-gas model do not diffuse independently. Having noted this, we propose to use the exact results for the anisotropic random walkers to rationalize the crossover behavior of the driven lattice gas. In the lattice-gas model, the E field at the edges sets up a density gradient which makes the diffusion of the individual particles asymmetric. Only the case $E=0$ corresponds to a symmetric random walk. The lifetime distribution of the particles introduced at, say, the edge $x=1$ is to a good approximation[13] given by

$$D(t)=D(t,-1)+D(t,L)\ . \quad (7)$$

The main contribution to the scaling region seen in Figs. 1 and 3 comes from $D(t,-1)$, whereas the broad-peak contribution at large t is produced by $D(t,L)$. When E is increased, the contribution to $D(t)$ from $D(t,-1)$ decreases and $D(t)$ eventually becomes determined by $D(t,L)$ which changes into a Gaussian centered around a characteristic time, $t=(L/\langle s\rangle)\delta t$. As the scaling regime vanishes, this Gaussian makes the power spectrum behave as $S(f)\sim 1/f^2$. The vanishing of the scaling region with increasing E, as seen on Fig. 3, is the effect of the vanishing of the scaling interval of $D(t,-1)$ as discussed above.

In conclusion, we have studied the particle-number fluctuations and the lifetime distribution in a finite-driven diffusive lattice gas. We find that, independent of the type of interaction, the temperature, and the spatial dimension, the power spectrum and lifetime distribution behave as if the particles on the lattice were independent random walkers. In the case of vanishing drive, this leads to scaling exponents, $\alpha\simeq 1.5$ and $\beta\simeq 1.5$. These exponents are different from the exponents found for the deterministic lattice gas of flux flow[2] which has $\alpha\simeq 2$ and $\beta\simeq 1$. When the flux-flow model is associated with stochastic dynamics, there is a crossover from $\beta\simeq 1$ to $\beta\simeq 1.5$. We want to argue that the difference between the $1/f^{3/2}$ power spectrum found in the present paper and the $1/f$ spectrum reported in Ref. 2 is due to the difference in the microscopic dynamics. The two models are very similar and the only significant difference in their definition is in the stochastic versus deterministic dynamics. Hence, we conclude that the stochastic nature of the diffusive dynamics is a relevant model property. When a characteristic time scale is introduced in the stochastic dynamics, there is a crossover to $(1/f^2)$-noise behavior.

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[1] P. Bak, C. Tang, and K. Wiesenfeld, Phys. Rev. Lett. **59**, 381 (1987); Phys. Rev. A **38**, 364 (1988).

[2] H. J. Jensen, Phys. Rev. Lett. **64**, 3103 (1990). See also H. J. Jensen, Mod. Phys. Lett. B (to be published), in which a more isotropic version of the lattice gas is discussed and where the result $\beta\simeq 1$ in both one and two dimensions is reported.

[3] C. Roland and M. Grant, Phys. Rev. Lett. **63**, 551 (1989).

[4] J. V. Andersen and O. G. Mouritsen, Phys. Rev. Lett. **65**, 440 (1990).

[5] J. V. Andersen and O. G. Mouritsen, in *Phase Transitions in Soft Condensed Matter,* edited by T. Riste and D. Sherrington (Plenum, New York, 1989), p. 343; J. V. Andersen and O. G. Mouritsen, Phys. Scr. **T33**, 141 (1990).

[6] J. V. Andersen, H. Bohr, and O. G. Mouritsen, Phys. Rev. B **42**, 283 (1990).

[7] S. Katz, J. L. Lebowitz, and H. Spohn, J. Stat. Phys. **34**, 497 (1984).

[8] For a recent review on driven diffusive systems, see B. Schmittmann, Int. J. Mod. Phys. B **4**, 2269 (1990).

[9] H. J. Jensen, K. Christensen, and H. C. Fogedby, Phys. Rev. B **40**, 7425 (1989).

[10] Due to the use of rather large system sizes in the present work, the statistics of the broad-peak contribution in Fig. 4 are relatively poor.

[11] The power spectrum of the total number of particles has recently been discussed using diffusion equations by several authors. G. Grinstein, T. Hwa, and H. J. Jensen (unpublished) considered the ordinary diffusion equation $dn/dt=\gamma\Delta n$ driven from the boundary including nonlinear terms both with and without conserving bulk noise. H. J. Jensen [Phys. Scr. (to be published)] treated the diffusion equation driven by a white-noise boundary condition. A $1/f$ spectrum is obtained when the diffusion equation is driven from the boundary. Inclusion of conserved bulk noise changes the spectrum to $1/f^{3/2}$. Nonlinear terms do not change this result. H. C. Fogedby, M. H. Jensen, Y.-C. Zhang, T. Bohr, H. J. Jensen, and H. H. Rugh (unpublished) considered the diffusion equation from the point of view of random walkers, i.e., including the conserving-noise term.

[12] W. Feller, *An Introduction to Probability Theory and Its Applications* (Wiley, New York, 1957), Vol. 1, Chap. XIV.

[13] Strictly speaking, one should obtain $D(t)$ by solving the problem of the first passage to one boundary with the presence of the other. This will give corrections to the expression in Eq. (7). However, these corrections are exponentially small in the linear size of the system. This is easily realized by the method of images which can be applied in the case when $\langle s\rangle=0$. Hence, the qualitative behavior of the distribution of lifetimes is not effected by these corrections.